Electron transport through a quantum wire coupled with a mesoscopic ring

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Abstract

Electronic transport through a quantum wire sandwiched between two metallic electrodes and coupled to a quantum ring, threaded by a magnetic flux ϕ, is studied. An analytic approach for the electron transport through the bridge system is presented based on the tight-binding model. The transport properties are discussed in three aspects: (a) presence of an external magnetic filed, (b) strength of the wire to electrode coupling, and (c) presence of in-plane electric field.

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1 Introduction

With the advancement in nanoscience and nanotechnology, the fabrication of sub-micron devices has become possible and has allowed one to study the electron transport through quantum systems in a very controllable way. These quantum systems have attracted much more attention since they constitute promising building blocks for future generation of electronic devices and directed attention on the study of discrete structures, such as a single molecule, arrays of molecules, quantum dots, quantum wires and mesoscopic rings. The electron transport through a bridge system was first studied theoretically in 1974 [1]. Later, several numerous experiments [2, 3, 4, 5, 6] have been performed through quantum systems placed between two metallic electrodes with few nanometer separation. The operation of such two-terminal devices is due to an applied bias. Current passing across the junction is strongly nonlinear function of applied bias voltage and its detailed description is a very complex problem. Though lot of theoretical as well as experimental papers have been available in the literature, yet the complete knowledge of the conduction mechanism in this scale is not well understood even today. The transport properties of these systems are associated with some quantum effects like, quantization of energy levels, quantum interference of electron waves, etc. A quantitative understanding of the physical mechanisms underlying the operation of nanoscale devices remains a major challenge in the present nanoelectronics research.

The aim of the present article is to reproduce an analytic approach based on the tight-binding model to investigate the electronic transport properties through a quantum wire coupled to a mesoscopic ring. There exist some *ab initio* methods for the calculation of conductance [7, 8, 9, 10, 11, 12], yet it is needed the simple parametric approaches [13, 14, 17, 15, 16, 18, 19, 20, 21, 22, 23] for this calculation, especially for the case of larger molecular bridge systems. The parametric study is motivated by the fact that the *ab initio* theories are computationally too expensive and here we focus our attention on the qualitative effects rather than the quantitative ones. This is why we restrict our calculations on the simple analytical formulation of the transport problem.

We organize the paper as follow. Following the introduction (Section 1), in Section 2, we present the model system under consideration and give a very brief description for the calculation of conductance and current-voltage characteristics through the bridge system. Section 3 presents the results of the system taken into account. Finally, we summarize our results in Section 4.

2 The model and a brief description onto the theoretical formulation

We begin by referring to Fig. 1. The system considered here is a quantum wire coupled to a mesoscopic ring with N atomic sites and the wire is attached to two semi-infinite one-dimensional (1D) metallic electrodes, namely, source and drain. The
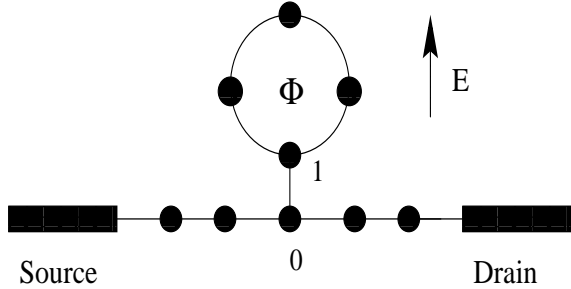

Figure 1: Schematic view of a quantum wire coupled to a mescopic ring, threaded by a magnetic flux ϕ, and the wire is attached to two 1D metallic electrodes.

full system (quantum wire with ring) is described by a single-band tight-binding Hamiltonian within a non-interacting electron picture, and it can be written in the form,

$$H_C = H_W + H_R + H_{WR} \qquad (1)$$

where, H_W, H_R and H_{WR} correspond to the Hamiltonians for the wire, ring and wire-to-ring coupling, respectively, and they can be expressed as,

$$H_W = \sum_i \epsilon_i d_i^\dagger d_i + \sum_{<ij>} t_w \left(d_i^\dagger d_j + d_j^\dagger d_i \right) \qquad (2)$$

$$H_R = \sum_k \epsilon_k c_k^\dagger c_k + \sum_{<kl>} t_r \left(c_k^\dagger c_l e^{i\theta} + c_l^\dagger c_k e^{-i\theta} \right) \qquad (3)$$

$$H_{WR} = t_0 \left(c_1^\dagger d_0 + d_0^\dagger c_1 \right) \qquad (4)$$

Here, ϵ_i's (ϵ_k's) are the on-site energies of the ring (wire), $d_i^\dagger$ and $c_k^\dagger$ are the creation operators of an electron at site i and k in the wire and ring. $\theta =$

$2\pi\phi/N$ is the phase factor due to the flux ϕ threaded by the ring. t_w (t_r) is the hopping integral between two nearest-neighbor sites in the ring (wire) and t_0 is the wire-to-ring tunneling coupling.

At much low temperatures and bias voltage, the linear conductance of the wire-ring system can be calculated by using one-channel Landauer conductance formula,

$$g = \frac{2e^2}{h}T \qquad (5)$$

where T is the transmission probability of an electron from the source to drain through the wire including the ring, and it is defined as [24],

$$T(E,V) = \text{Tr}\left[(\Sigma_S^r - \Sigma_S^a)\, G^r\, (\Sigma_D^a - \Sigma_D^r)\, G^a\right] \quad (6)$$

Now the Green's function G of the full system (wire with ring) is given by the relation,

$$G = [E - H_C - \Sigma_S - \Sigma_D]^{-1} \qquad (7)$$

where E is the energy of injecting electrons from the source and H is the Hamiltonian of the full system described above (Eq. 1). In Eq. 7, $\Sigma_S = h_{SC}^\dagger g_S h_{SC}$ and $\Sigma_D = h_{DC} g_D h_{DC}^\dagger$, are the self-energy terms due to the two electrodes. g_S and g_D correspond to the Green's functions for the source and drain, respectively. h_{SC} and h_{DC} are the coupling matrices and they are non-zero only for the adjacent points of the quantum wire and the electrodes. The coupling terms Γ_S and Γ_D for the full system can be calculated through the expression [24],

$$\Gamma_{\{S,D\}} = i\left[\Sigma_{\{S,D\}}^r - \Sigma_{\{S,D\}}^a\right] \qquad (8)$$

where $\Sigma_{\{S,D\}}^r$ and $\Sigma_{\{S,D\}}^a$ are the retarded and advanced self-energies respectively and they are conjugate to each other. Datta *et al.* [25] have shown that the self-energies can be expressed like,

$$\Sigma_{\{S,D\}}^r = \Lambda_{\{S,D\}} - i\Delta_{\{S,D\}} \qquad (9)$$

where $\Lambda_{\{S,D\}}$ are the real parts of the self-energies which correspond to the shift of the energy eigenvalues of the full system (quantum wire with ring) and the imaginary parts $\Delta_{\{S,D\}}$ of the self-energies represent the broadening of the energy levels. Since this broadening is much larger than the thermal broadening, we restrict our all calculations only at absolute zero temperature. By doing some simple calculations, these real and imaginary parts of the self-energies can be determined in terms of the coupling strength ($\tau_{\{S,D\}}$) between the wire and two electrodes, injecting electron energy (E) and hopping strength (v) between nearest-neighbor sites in

the electrodes. Using Eq. 9, the coupling terms Γ_S and Γ_D can be written in terms of the retarded self-energy as,

$$\Gamma_{\{S,D\}} = -2\text{Im}\left[\Sigma_{\{S,D\}}^r\right] \qquad (10)$$

All the information regarding the wire to electrode coupling are included into the two self energies stated above and is analyzed through the use of Newns-Anderson chemisorption theory [13, 14]. The detailed description of this theory is obtained in these two references.

Thus, by calculating the self-energies, the coupling terms Γ_S and Γ_D can be easily obtained and then the transmission probability T will be calculated from the expression given in Eq. 6.

The current passing through the bridge is depicted as a single-electron scattering process between the two reservoirs of charge carriers. The current-voltage relation is evaluated from the following expression [24],

$$I(V) = \frac{e}{\pi\hbar} \int\limits_{E_F - eV/2}^{E_F + eV/2} T(E,V)\, dE \qquad (11)$$

where E_F is the equilibrium Fermi energy. For the sake of simplicity, here we assume that the entire voltage is dropped across the wire-electrode interfaces and this assumption does not greatly affect the qualitative aspects of the *I-V* characteristics. Throughout the article we set E_F to 0 and use the units $c = e = h = 1$.

3 Results and discussion

Here we describe conductance-energy and current-voltage characteristics through the quantum wire coupled to a mesoscopic ring at absolute zero temperature. Electron transport properties through the system are strongly affected by the magnetic flux ϕ, wire-to-electrode coupling strength and the in-plane electric field. In the presence of in-plane electric filed and assuming it along the perpendicular direction of the wire, the dependence of the site energies on the electric field $\mathcal{E}$ is written within the tight-binding approximation as [15],

$$\begin{aligned} \epsilon_i &= (e\mathcal{E}aN/2\pi)\cos\left[2\pi(i-1)/N\right] \\ &= (et_r)(\mathcal{E}^\star N/2\pi)\cos\left[2\pi(i-1)/N\right] \quad (12) \end{aligned}$$

where, a is lattice spacing in the mesoscopic ring and $\mathcal{E}^\star$ is the dimensionless electric field strength

defined by $\mathcal{E}a/t_r$. For simplicity, here we assume t_w, t_r and t_0 are identical to each other in magnitude and specify them by the symbol t. We investigate all the essential features of electron transport for the two limiting cases. One is the weak-coupling limit, defined as $\tau_{\{S,D\}} \ll t$ and the other one is the strong-coupling limit and defined
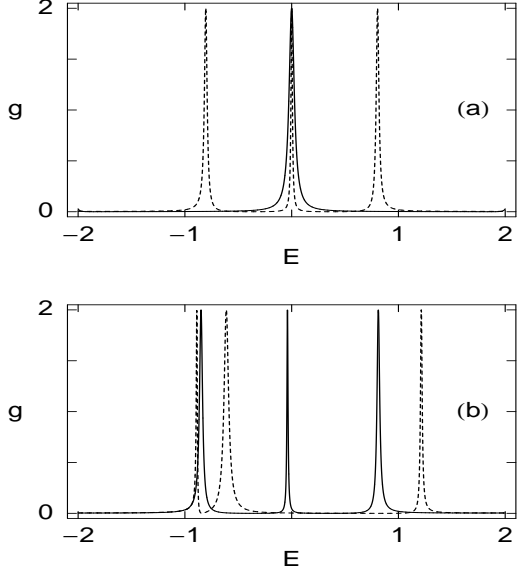

Figure 2: Conductance g as a function of energy E in the weak-coupling limit for the system with ring size $N = 10$, where (a) in the absence of any electric filed with $\phi = 0$ (solid line) and 0.4 (dotted line) and (b) in the presence of $\phi = 0.4$ with $\mathcal{E} = 2$ (solid line) and 4 (dotted line).

it as $\tau_{\{S,D\}} \sim t$. The parameters τ_S and τ_D correspond to the couplings of the wire to the source and drain, respectively. The common set of values of these parameters in the two limiting cases are as follow: $\tau_S = \tau_D = 0.5$, $t = 3$ (weak-coupling) and $\tau_S = \tau_D = 2$, $t = 3$ (strong-coupling).

In Fig. 2, we plot the conductance (g) as a function of the injecting electron energy (E) for the bridge system in the limit of weak-coupling. Figure 2(a) corresponds to the spectrum in the absence of any electric filed where, the solid and dotted curves are respectively for $\phi = 0$ and 0.4. In Fig. 2(b), the spectrum is shown for the non-zero value of the electric field with $\phi = 0.4$ where, the solid and dotted curves represent the results for the electric filed strengths $\mathcal{E} = 2$ and 4, respectively. Conductance vanishes almost for all energies except at resonances where it approaches to 2.

At these resonances, the transmission probability T becomes unity, since $g = 2T$ (from the Landauer formula with $e = h = 1$). The resonant peaks in the conductance spectrum coincide with eigenenergies of the system (wire including the ring), and thus the spectrum manifests itself the energy levels of the system. For zero electric field strength and in the absence of magnetic flux ϕ, the conductance exhibits a single resonant peak across $E = 0$ (see solid curve of Fig. 2(a)), while, in the presence of ϕ more resonant peaks appear in the spectrum (see dotted curve of Fig. 2(a)). It reveals that for non-zero value of ϕ more resonating states appear in the system. This is due to the removal of all the degeneracies in the energy eigenstates for any non-zero value of ϕ. In the presence of in-plane electric field, these resonant peaks are shifted and the conductance spectrum becomes asymmetric with respect to the energy E (see Fig. 2(b)).

For the strong wire-to-electrode coupling, resonant peaks get substantial widths as presented in Fig. 3 where, the solid and dotted curves correspond
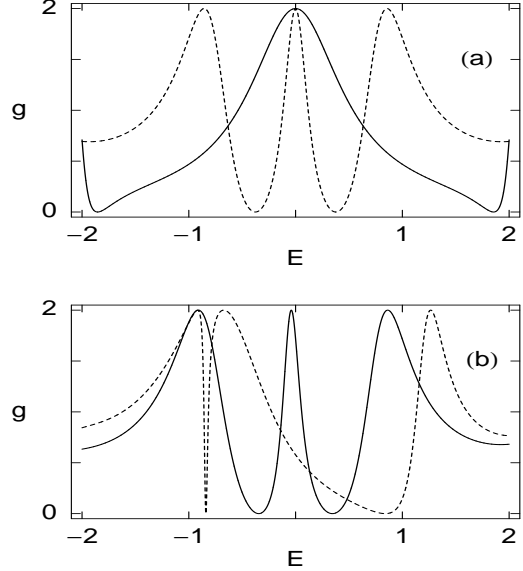

Figure 3: Conductance g as a function of energy E in the strong-coupling limit for the system with ring size $N = 10$, where (a) in the absence of any electric filed with $\phi = 0$ (solid line) and 0.4 (dotted line) and (b) in the presence of $\phi = 0.4$ with $\mathcal{E} = 2$ (solid line) and 4 (dotted line).

to the identical meaning as earlier. The increment of the resonant widths is due to the broadening of the energy levels of the wire including the ring,

where the contribution comes from the imaginary parts of the two self-energies [24].

The scenario of electron transfer through the bridge becomes much more clearly visible by studying the current I as a function of the applied bias voltage V. The Current is computed from the in-
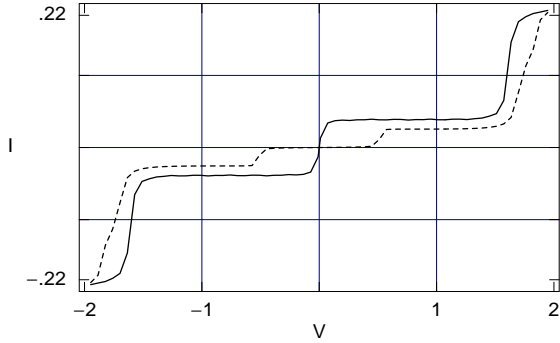

Figure 4: Current I as a function of bias voltage V in the limit of weak wire-to-electrode coupling for the system with ring size $N = 10$ and $\phi = 0.4$. The solid and dotted lines correspond to the currents for $\mathcal{E} = 0$ and 3, respectively.

tegration procedure of the transmission function T which shows the same variation, differ only in magnitude by the factor 2, like as the conductance spec-
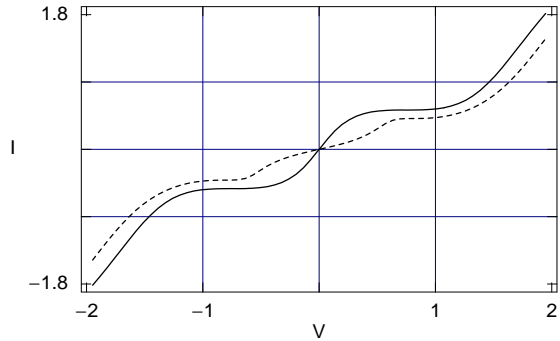

Figure 5: Current I as a function of bias voltage V in the limit of strong wire-to-electrode coupling for the system with ring size $N = 10$ and $\phi = 0.4$. The solid and dotted curves correspond to the currents for $\mathcal{E} = 0$ and 3, respectively.

tra (Figs. 2 and 3). The current-voltage characteristic in the weak-coupling limit for the bridge system is shown in Fig. 4 where, the solid curve corresponds to the current in the absence of any electric field and the dotted curve denotes the same for $\mathcal{E} = 3$. Here we take $\phi = 0.4$. The current shows staircase-like behavior with sharp steps, which is associated

with the discrete nature of the resonant spectrum (Fig. 2). The shape and width of the current steps depend on the width of the resonant spectrum since the hight of a step in I-V curve is directly proportional to the area of the corresponding peak in the conductance spectrum. On the other hand, the current varies continuously with the applied bias voltage and achieves much bigger values in the strong-coupling limit, as shown in Fig. 5 where, the solid and dotted curves correspond to the same meaning as earlier. From both Figs. 4 and 5 it is clearly observed that the in-plane electric field suppresses the current amplitude (see the dotted curves). This feature may be utilized to control *externally* the amplitude of the current through the bridge system.

4   Concluding remarks

To summarize, we have introduced parametric approach based on the tight-binding model to investigate the electron transport properties at absolute zero temperature through a quantum wire coupled to a mesoscopic ring threaded by a magnetic flux ϕ. A simple parametric approach is given to study electron transport properties through the system, and it can be used to study the transport behavior in any complicated molecular bridge system. Electronic conduction through the quantum wire is strongly influenced by the flux ϕ threaded by the ring and the wire-to-electrode coupling strength. The effects of in-plane electric field have also been studied in this context and it has been predicted that the current amplitude can be controlled *externally* through the bridge system by means of this electric field.

References

[1] A. Aviram and M. Ratner, Chem. Phys. Lett. **29**, 277 (1974).

[2] R. M. Metzger *et al.*, J. Am. Chem. Soc. **119**, 10455 (1997).

[3] C. M. Fischer, M. Burghard, S. Roth and K. V. Klitzing, Appl. Phys. Lett. **66**, 3331 (1995).

[4] J. Chen, M. A. Reed, A. M. Rawlett and J. M. Tour, Science **286**, 1550 (1999).

[5] M. A. Reed, C. Zhou, C. J. Muller, T. P. Burgin and J. M. Tour, Science **278**, 252 (1997).

[6] R. H. M. Smit, C. Untiedt, G. Rubio-Bollinger, R. C. Segers and J. M. van Ruitenbeek, Phys. Rev. Lett. **91**, 076805 (2003).

[7] S. N. Yaliraki, A. E. Roitberg, C. Gonzalez, V. Mujica and M. A. Ratner, J. Chem. Phys. **111**, 6997 (1999).

[8] M. Di Ventra, S. T. Pantelides and N. D. Lang, Phys. Rev. Lett. **84**, 979 (2000).

[9] Y. Xue, S. Datta and M. A. Ratner, J. Chem. Phys. **115**, 4292 (2001).

[10] J. Taylor, H. Gou and J. Wang, Phys. Rev. B **63**, 245407 (2001).

[11] P. A. Derosa and J. M. Seminario, J. Phys. Chem. B **105**, 471 (2001).

[12] P. S. Damle, A. W. Ghosh and S. Datta, Phys. Rev. B **64**, R201403 (2001).

[13] V. Mujica, M. Kemp and M. A. Ratner, J. Chem. Phys. **101**, 6849 (1994).

[14] V. Mujica, M. Kemp, A. E. Roitberg and M. A. Ratner, J. Chem. Phys. **104**, 7296 (1996).

[15] P. A. Orellana, M. L. Ladron de Guevara, M. Pacheco and A. Latge, Phys. Rev. B **68**, 195321 (2003).

[16] P. A. Orellana, F. Dominguez-Adame, I. Gomez and M. L. Ladron de Guevara, Phys. Rev. B **67**, 085321 (2003).

[17] M. P. Samanta, W. Tian, S. Datta, J. I. Henderson and C. P. Kubiak, Phys. Rev. B **53**, R7626 (1996).

[18] M. Hjort and S. Staftröm, Phys. Rev. B **62**, 5245 (2000).

[19] R. Baer and D. Neuhauser, Chem. Phys. **281**, 353 (2002).

[20] R. Baer and D. Neuhauser, J. Am. Chem. Soc. **124**, 4200 (2002).

[21] D. Walter, D. Neuhauser and R. Baer, Chem. Phys. **299**, 139 (2004).

[22] K. Walczak, Cent. Eur. J. Chem. **2**, 524 (2004).

[23] K. Walczak, Phys. Stat. Sol. (b) **241**, 2555 (2004).

[24] S. Datta, *Electronic transport in mesoscopic systems*, Cambridge University Press, Cambridge 1997.

[25] W. Tian, S. Datta, S. Hong, R. Reifenberger, J. I. Henderson and C. I. Kubiak, J. Chem. Phys. **109**, 2874 (1998).